Mrs Fuller

83586

Access DB# _____

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: BEN DACKEY Examiner #: 73499 Date: 1/4/03
Art Unit: 1626 Phone Number 30 5-6589 Serial Number: 10/072,600
Mail Box and Bldg/Room Location: CM1 3611 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

****

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

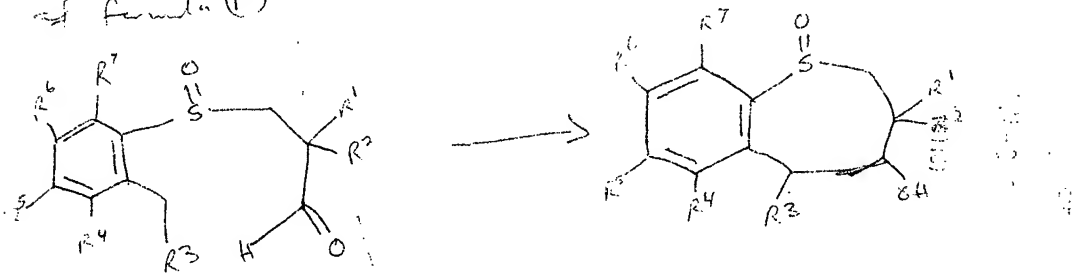
Title of Invention: Method for preparing a stereoselectively enriched dihydrobenzothiepine

Inventors (please provide full names): Li et al.

Earliest Priority Filing Date: 12/19/97

***For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.**

A method of cyclizing and enantiomerically enriched aryl-3-propanal sulfoxide of formula (II) to produce dihydrobenzothiepine-1-oxide of formula (I)



The cyclizing step is performed in the presence of a base especially potassium t-butoxide

Point of Contact:
Thomas G. Larson, Ph.D.
703-308-7309
CM1, Rm. 6 B 01

****

STAFF USE ONLY

Searcher: TGL
Searcher Phone #: _____
Searcher Location: _____
Date Searcher Picked Up: 1/8/03
Date Completed: 1/10/03
Searcher Prep & Review Time: 60
Clerical Prep Time: _____
Online Time: 91

Type of Search

NA Sequence (#) _____
AA Sequence (#) _____
Structure (#) 2
Bibliographic _____
Litigation _____
Fulltext _____
Patent Family _____
Other Rxn

Vendors and cost where applicable

STN $ 551
Dialog _____
Questel/Orbit _____
Dr.Link _____
Lexis/Nexis _____
Sequence Systems _____
WWW/Internet _____
Other (specify) _____

PTO-1590 (8-01)

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=> file reg caplus
FILE 'REGISTRY' ENTERED AT 14:04:06 ON 10 JAN 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2003 American Chemical Society (ACS)

FILE 'CAPLUS' ENTERED AT 14:04:06 ON 10 JAN 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

=> d que l16
L3                  STR
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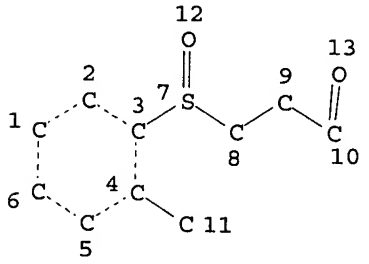


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NODE ATTRIBUTES:
CONNECT IS E3  RC AT   7
CONNECT IS E2  RC AT  10
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  13

STEREO ATTRIBUTES: NONE
L5                  STR
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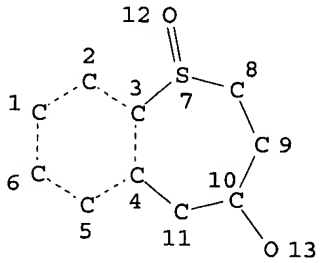
Non-H connections limited to 3 @ node 7 to avoid picking up $-\overset{\overset{O}{\|}}{\underset{\underset{O}{\|}}{S}}-$.

Non-H connections limited to exactly 2 @ 10 so that aldehydes but not ketones are picked up.

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NODE ATTRIBUTES:
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CONNECT IS E1  RC AT  13
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  13

STEREO ATTRIBUTES: NONE
L11             5 SEA FILE=REGISTRY SSS FUL L5
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see reason above.

Non-H connections limited to 1 @ 13 so that hydroxyl groups are picked up, but not ether and ester groups.

Search structure L5 in Registry file

```
L13          5 SEA FILE=REGISTRY SSS FUL L3
L14          4 SEA FILE=CAPLUS ABB=ON  PLU=ON  L11
L15          4 SEA FILE=CAPLUS ABB=ON  PLU=ON  L13
L16          3 SEA FILE=CAPLUS ABB=ON  PLU=ON  L14 AND L15
```

Search L3 in Reg. } search CAPLUS file with hit structures in Registry - look for documents in CAPLUS having both structures.

=> D IBIB ABS HITSTR l16 1-3

L16 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2000:590035 CAPLUS
DOCUMENT NUMBER: 133:193089
TITLE: Preparation of substituted 5-aryl-benzothiepines as ileal bile acid transport and taurocholate uptake inhibitors
INVENTOR(S): Lee, Len F.; Banerjee, Shyamal C.; Huang, Horng-chih; Li, Jinglin J.; Miller, Raymond E.; Reitz, David B.; Tremont, Samuel J.
PATENT ASSIGNEE(S): G.D. Searle and Co., USA
SOURCE: U.S., 191 pp., Cont.-in-part of U. S. Ser. No. 109,551.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 8
PATENT INFORMATION:

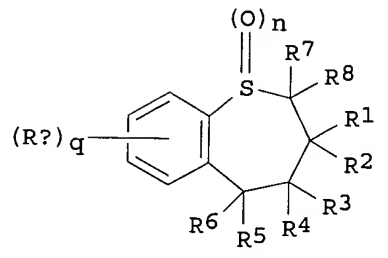
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6107494	A	20000822	US 1999-275463	19990324
US 5994391	A	19991130	US 1998-109551	19980702
CA 2336315	AA	20000113	CA 1999-2336315	19990629
WO 2000001687	A1	20000113	WO 1999-US12828	19990629
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9948202	A1	20000124	AU 1999-48202	19990629
EP 1091953	A1	20010418	EP 1999-931769	19990629
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 9911737	A	20011211	BR 1999-11737	19990629
JP 2002519418	T2	20020702	JP 2000-558091	19990629
US 6262277	B1	20010717	US 1999-443403	19991119
NO 2001000016	A	20010302	NO 2001-16	20010102
US 2002013476	A1	20020131	US 2001-828968	20010409
US 6387924	B2	20020514		
US 2002188119	A1	20021212	US 2002-72600	20020211

PRIORITY APPLN. INFO.:

US 1994-305526	B2	19940913
US 1995-517051	B1	19950821
US 1996-13119P	P	19960311
US 1997-816065	B2	19970311
US 1997-831284	B2	19970331
US 1997-68170P	P	19971219
US 1998-109551	A2	19980702
US 1999-275463	A1	19990324

WO 1999-US12828 W 19990629
US 1999-443403 A1 19991119
US 2000-581897 A3 20001002

OTHER SOURCE(S): MARPAT 133:193089
GI



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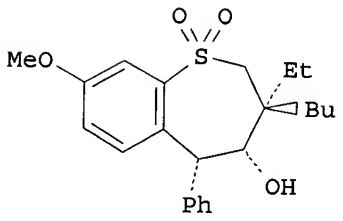
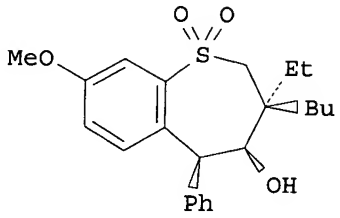


II



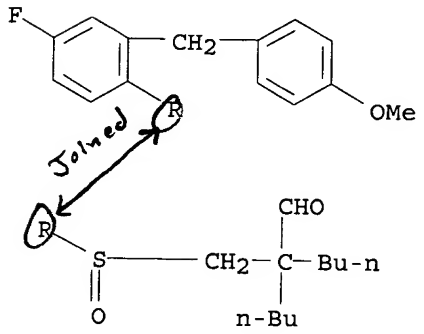
III

AB The title compds. (I) [wherein q = 1-4; n = 2; R1 and R2 = independently H or (un)substituted (halo)alkyl, alkenyl, alkynyl, alkylaryl, arylalkyl, alkoxy(alkyl), dialkylamino, alkylthio, (polyalkyl)aryl, or cycloalkyl; or R1 and R2 taken together with the atoms to which they are attached = cycloalkyl; R3 and R4 = independently H, alkyl, alkenyl, alkynyl, acyloxy, aryl, heterocyclyl, OR9, NR9R10, SR9, S(O)R9, SO2R9, or SO3R9; R9 and R10 = independently H, (cyclo)alkyl, alkenyl, alkynyl, aryl(alkyl), acyl, heterocyclyl, or ammoniumalkyl; or R3 and R4 together = :O, :NOR11, :S, :NNR11R12, :NR9, or :CR11R12; R11 and R12 = independently H, (cyclo)alkyl, alkenyl, alkynyl, aryl(alkyl), heterocyclyl, carboxylalkyl, carboalkoxyalkyl, cyanoalkyl, OR9, NR9R10, SR9, S(O)R9, SO2R9, SO3R9, CO2R9, CN, halo, oxo, or CONR9R10; R5 = substituted aryl; R6 = H; R7 and R8 = independently H or alkyl; Rx = independently H or (un)substituted (cyclo)alkyl, alkenyl, alkynyl, polyalkyl, acyloxy, aryl(alkyl), halo(alkyl), (quaternary) heterocyclyl, (quaternary) heteroaryl, polyether, alkoxy, amino, alkylthio, NO2, carboxy, carbamido, etc.] where prepd. for the prophylaxis and treatment of hyperlipidemic conditions, such as those assocd. with atherosclerosis or hypercholesterolemia. Thus, KOBu-t was added to a soln. of 2-((2-benzyl-5-methoxyphenylsulfonyl)methyl)-2-ethylhexanal (prepn. given) and dry THF cooled to -1.6.degree.C to give, after workup, II and III (96% combined yield). The isomers were sepd. upon recrystn. II inhibited IBAT-mediated uptake of [14C]-taurocholate in H14 cells with an IC50 of 0.1 .mu.M and reduced serum cholesterol from 143 mg (7%) to 126 mg (2%) compared to control in cholesterol-fed hamsters in a 14-day test. In vitro taurocholate uptake assay data are included for nearly 600 compds. of the invention.

IT **228113-61-9P 228113-62-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of substituted 5-aryl-benzothiepines by cyclization of 2-((2-benzyl- and 2-benzoylphenylthio)methyl)alkanals as ileal bile acid transport and taurocholate uptake inhibitors)

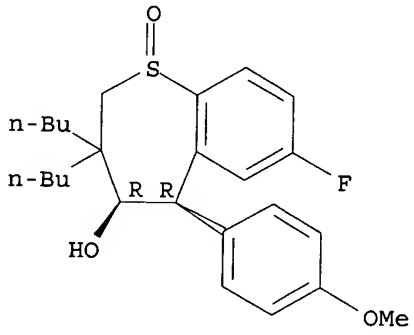
RN 228113-61-9 CAPLUS
CN Hexanal, 2-butyl-2-[[[4-fluoro-2-[(4-methoxyphenyl)methyl]phenyl]sulfinyl]methyl]- (9CI) (CA INDEX NAME)



single structure

RN 228113-62-0 CAPLUS
CN 1-Benzothiepin-4-ol, 3,3-dibutyl-7-fluoro-2,3,4,5-tetrahydro-5-(4-methoxyphenyl)-, 1-oxide, (4R,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2000:229073 CAPLUS
DOCUMENT NUMBER: 133:4591
TITLE: A highly enantioselective benzothiepine synthesis
AUTHOR(S): Wang, Ching-Cheng; Li, James J.; Huang, Horng-Chih; Lee, Len F.; Reitz, David B.
CORPORATE SOURCE: Medicinal Chemistry Searle Research Development, Monsanto Company, St. Louis, MO, 63017, USA
SOURCE: Journal of Organic Chemistry (2000), 65(9), 2711-2715
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:4591
GI

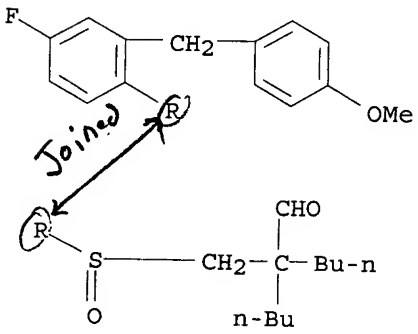
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB A highly enantioselective synthesis of benzothiepine I has been accomplished via an enantioenriched sulfoxide intermediate II (R = CH2OH) obtained by asym. oxidn. with a chiral oxaziridine in 89:11 er. The key step is a thermodynamically controlled asym. cyclization reaction of methoxybenzylphenyl-.beta.-sulfinyl aldehyde II (R = CHO) that produces two new stereogenic centers. The (4R,5R) isomer I was obtained in 98:2 er. Treatment of racemic benzothiazepine III (R1 = H; R2 = HO) and its epimer III (R1 = HO; R2 = H) to the cyclization conditions (KOCMe3, -10.degree. in THF) gives a 77:23 mixt. of stereoisomers favoring III (R1 = H; R2 = HO), indicating that the stereoselective formation of III occurs by a thermodn. process whose diastereoselectivity is controlled by the sulfoxide configuration.

IT **228113-61-9P 270931-14-1P 270931-15-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(enantioselective synthesis of a benzothiepine intermediate in the prepn. of an apical sodium bile acid transporter inhibitor by stereoselective cyclization of a nonracemic benzylphenylsulfinyl aldehyde deriv.)

RN 228113-61-9 CAPLUS

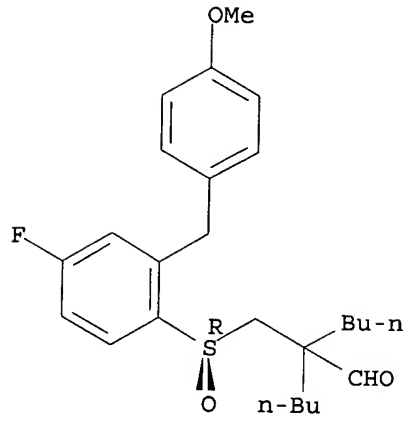
CN Hexanal, 2-butyl-2-[[[4-fluoro-2-[(4-methoxyphenyl)methyl]phenyl]sulfinyl]methyl]- (9CI) (CA INDEX NAME)



RN 270931-14-1 CAPLUS

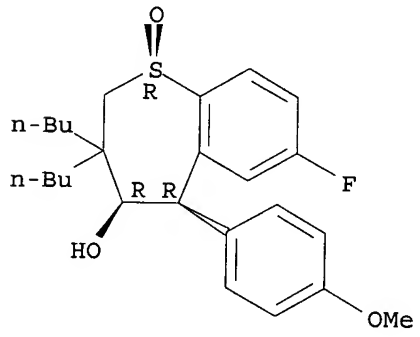
CN Hexanal, 2-butyl-2-[[(R)-[4-fluoro-2-[(4-methoxyphenyl)methyl]phenyl]sulfinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



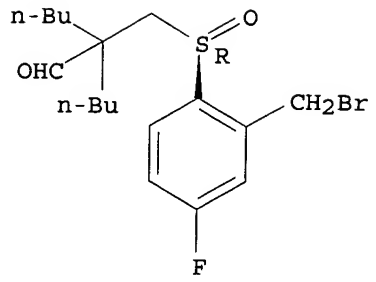
RN 270931-15-2 CAPLUS
CN 1-Benzothiepin-4-ol, 3,3-dibutyl-7-fluoro-2,3,4,5-tetrahydro-5-(4-methoxyphenyl)-, 1-oxide, (1R,4R,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



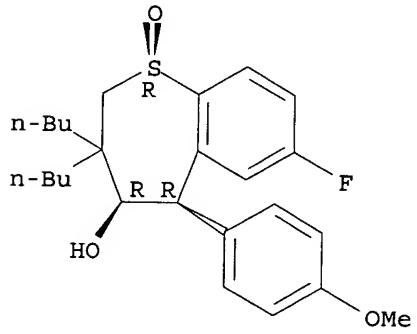
IT **270931-12-9P 270931-16-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective synthesis of a benzothiepine intermediate in the prepn. of an apical sodium bile acid transporter inhibitor by stereoselective cyclization of a nonracemic benzylphenylsulfinyl aldehyde deriv.)
RN 270931-12-9 CAPLUS
CN Hexanal, 2-[[(R)-[2-(bromomethyl)-4-fluorophenyl]sulfinyl]methyl]-2-butyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



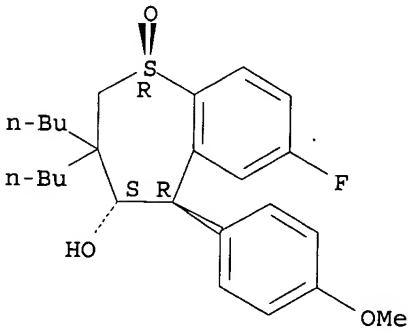
RN 270931-16-3 CAPLUS
CN 1-Benzothiepin-4-ol, 3,3-dibutyl-7-fluoro-2,3,4,5-tetrahydro-5-(4-methoxyphenyl)-, 1-oxide, (1R,4R,5R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



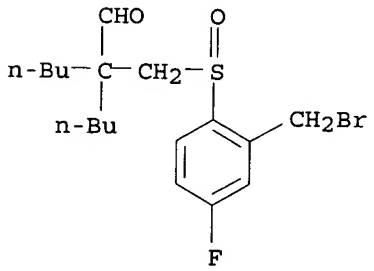
IT **270931-18-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(equilibration studies of stereoselective phenylbenzothiazepinol oxide prepn. by cyclization of a benzylphenylsulfinyl aldehyde)
RN 270931-18-5 CAPLUS
CN 1-Benzothiepin-4-ol, 3,3-dibutyl-7-fluoro-2,3,4,5-tetrahydro-5-(4-methoxyphenyl)-, 1-oxide, (1R,4S,5R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT **340166-91-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 340166-91-8 CAPLUS
CN Hexanal, 2-[[[2-(bromomethyl)-4-fluorophenyl]sulfinyl]methyl]-2-butyl-(9CI) (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1999:421680 CAPLUS
DOCUMENT NUMBER: 131:58769
TITLE: Preparation of enantiomerically-enriched tetrahydrobenzothiepine oxides by cyclization of arylpropanalsulfoxides.
INVENTOR(S): Li, James; Wang, Ching-Cheng; Reitz, David B.; Snieckus, Victor; Huang, Horng-Chih; Carpenter, Andrew J.
PATENT ASSIGNEE(S): G.D. Searle & Co., USA
SOURCE: PCT Int. Appl., 100 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 8
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9932478	A1	19990701	WO 1998-US26216	19981216
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9917213	A1	19990712	AU 1999-17213	19981216
EP 1042314	A1	20001011	EP 1998-962044	19981216
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
JP 2001526284	T2	20011218	JP 2000-525415	19981216
BR 9814300	A	20020205	BR 1998-14300	19981216
ZA 9811648	A	19991220	ZA 1998-11648	19981218
US 6369220	B1	20020409	US 2000-581897	20001002
US 2002188119	A1	20021212	US 2002-72600	20020211

PRIORITY APPLN. INFO.:
US 1997-68170P P 19971219
WO 1998-US26216 W 19981216
US 2000-581897 A3 20001002

OTHER SOURCE(S): CASREACT 131:58769; MARPAT 131:58769
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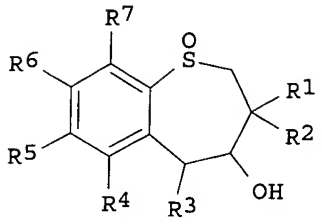

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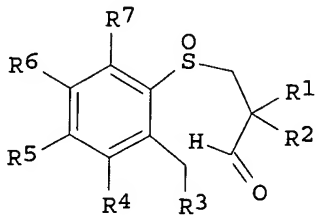


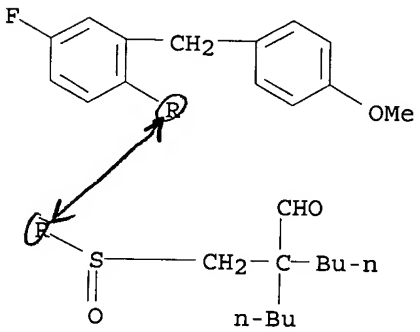
II

AB Title compds. [I; R1, R2 = H, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heteroaryl; R3 = H, (substituted) alkyl, alkenyl, alkynyl, aryl, cycloalkyl, heterocyclyl, etc.; R4-R7 = H, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heteroaryl, halo, alkoxy, aryloxy, NO2, amino; R3 and the OH are syn], were prepd. by cyclization of enantiomerically-enriched aldehydes (II; R1-R7 as above). Thus, enantiomerically-enriched II (R1, R2 = Bu; R4, R6, R7 = H; R5 = F; R3 = 4-MeOC6H4) (prepn. given) was stirred with KOCMe3 in THF at -15.degree. to give 77.7% (4R,5R)-I (variables as before).

IT **228113-61-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(enantiomerically-enriched; prepn. of enantiomerically-enriched tetrahydrobenzothiepine oxides by cyclization of arylpropanalsulfoxides)

RN 228113-61-9 CAPLUS

CN Hexanal, 2-butyl-2-[[[4-fluoro-2-[(4-methoxyphenyl)methyl]phenyl]sulfinyl]methyl]- (9CI) (CA INDEX NAME)



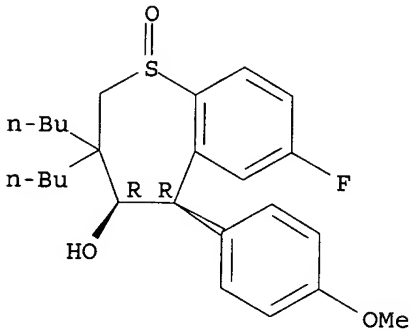
single structure

IT **228113-62-0P**
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of enantiomerically-enriched tetrahydrobenzothiepine oxides by cyclization of arylpropanalsulfoxides)

RN 228113-62-0 CAPLUS

CN 1-Benzothiepin-4-ol, 3,3-dibutyl-7-fluoro-2,3,4,5-tetrahydro-5-(4-methoxyphenyl)-, 1-oxide, (4R,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> FIL CASREACT
FILE 'CASREACT' ENTERED AT 14:17:50 ON 10 JAN 2003
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

FILE CONTENT:1907 - 5 Jan 2003 VOL 138 ISS 1

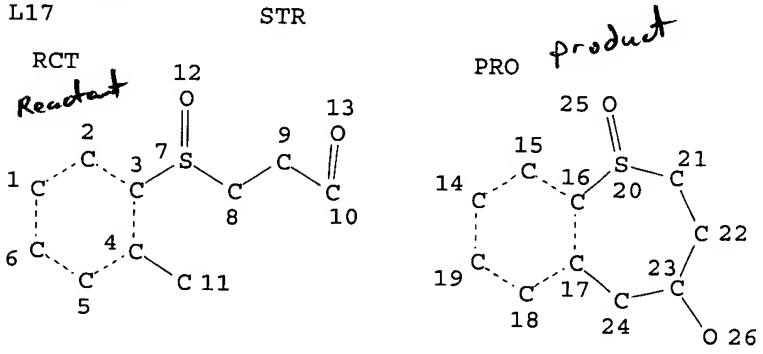
Some records from 1974 to 1991 are derived from the ZIC/VINITI data file and provided by InfoChem and some records are produced using some INPI data from the period prior to 1986.

This file contains CAS Registry Numbers for easy and accurate substance identification.

Crossover limits have been increased. See HELP RNCROSSOVER for details.

Structure search limits have been raised. See HELP SLIMIT for the new, higher limits.

=> d que
L17 STR



NODE ATTRIBUTES:

CONNECT IS E3 RC AT 7
CONNECT IS E2 RC AT 10
CONNECT IS E3 RC AT 20
CONNECT IS E1 RC AT 26
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

} Non-H connectivity limited for same reasons as in L3 & L5 above

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 26

STEREO ATTRIBUTES: NONE
L19 2 SEA FILE=CASREACT SSS FUL L17 (2 REACTIONS)

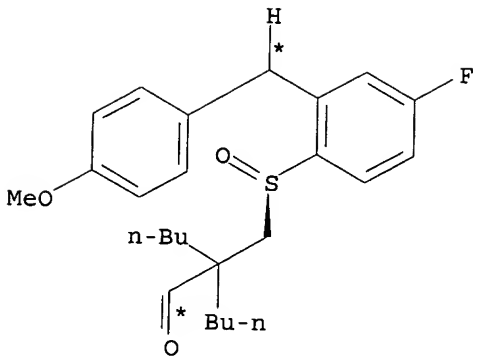
=> d bib abs hit 1-2

L19 ANSWER 1 OF 2 CASREACT COPYRIGHT 2003 ACS
AN 133:4591 CASREACT
TI A highly enantioselective benzothiepine synthesis
AU Wang, Ching-Cheng; Li, James J.; Huang, Horng-Chih; Lee, Len F.; Reitz, David B.
CS Medicinal Chemistry Searle Research Development, Monsanto Company, St. Louis, MO, 63017, USA
SO Journal of Organic Chemistry (2000), 65(9), 2711-2715
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

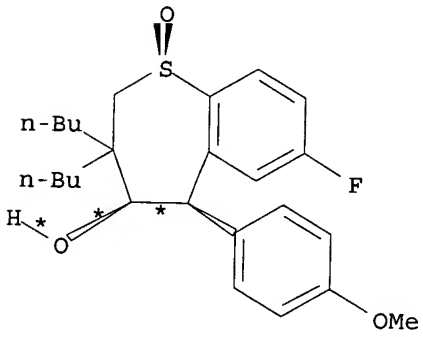
AB A highly enantioselective synthesis of benzothiepine I has been accomplished via an enantioenriched sulfoxide intermediate II (R = CH2OH) obtained by asym. oxidn. with a chiral oxaziridine in 89:11 er. The key step is a thermodynamically controlled asym. cyclization reaction of methoxybenzylphenyl-.beta.-sulfinyl aldehyde II (R = CHO) that produces two new stereogenic centers. The (4R,5R) isomer I was obtained in 98:2 er. Treatment of racemic benzothiazepine III (R1 = H; R2 = HO) and its epimer III (R1 = HO; R2 = H) to the cyclization conditions (KOCMe3, -10.degree. in THF) gives a 77:23 mixt. of stereoisomers favoring III (R1 = H; R2 = HO), indicating that the stereoselective formation of III occurs by a thermodn. process whose diastereoselectivity is controlled by the sulfoxide configuration.
RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(5) OF 17 ...K ===> S...



K

(5) →



S
YIELD 78%

RX(5) RCT K **270931-14-1**

STAGE(1)
RGT T 865-47-4 t-BuOK
SOL 109-99-9 THF

STAGE(2)
RGT G 7732-18-5 Water

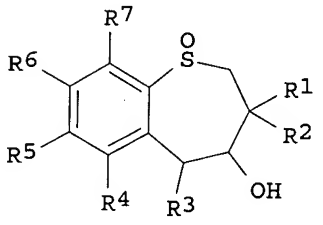
STAGE(3)
RGT U 7647-01-0 HCl
SOL 7732-18-5 Water
PRO S **270931-15-2**
NTE SIMILAR RESULTS FROM RACEMIC REACTANT

L19 ANSWER 2 OF 2 CASREACT COPYRIGHT 2003 ACS
AN 131:58769 CASREACT
TI Preparation of enantiomerically-enriched tetrahydrobenzothiepine oxides by cyclization of arylpropanalsulfoxides.
IN Li, James; Wang, Ching-Cheng; Reitz, David B.; Snieckus, Victor; Huang, Horng-Chih; Carpenter, Andrew J.

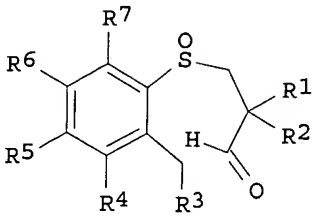
PA G.D. Searle & Co., USA
SO PCT Int. Appl., 100 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 8

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9932478	A1	19990701	WO 1998-US26216	19981216
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	AU 9917213	A1	19990712	AU 1999-17213	19981216
	EP 1042314	A1	20001011	EP 1998-962044	19981216
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
	JP 2001526284	T2	20011218	JP 2000-525415	19981216
	BR 9814300	A	20020205	BR 1998-14300	19981216
	ZA 9811648	A	19991220	ZA 1998-11648	19981218
	US 6369220	B1	20020409	US 2000-581897	20001002
	US 2002188119	A1	20021212	US 2002-72600	20020211
PRAI	US 1997-68170P	19971219			
	WO 1998-US26216	19981216			
	US 2000-581897	20001002			

OS MARPAT 131:58769
GI



I

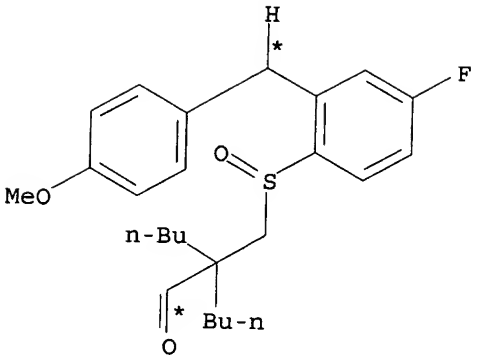


II

AB Title compds. [I; R1, R2 = H, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heteroaryl; R3 = H, (substituted) alkyl, alkenyl, alkynyl, aryl, cycloalkyl, heterocyclyl, etc.; R4-R7 = H, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heteroaryl, halo, alkoxy, aryloxy, NO2, amino; R3 and the OH are syn], were prepd. by cyclization of enantiomerically-enriched aldehydes (II; R1-R7 as above). Thus, enantiomerically-enriched II (R1, R2 = Bu; R4, R6, R7 = H; R5 = F; R3 = 4-MeOC6H4) (prepn. given) was stirred with KOCMe3 in THF at -15.degree. to give 77.7% (4R,5R)-I (variables as before).

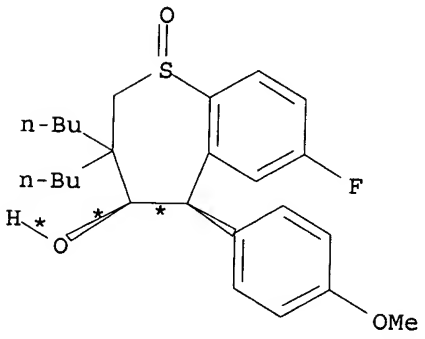
RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(3) OF 6 ...**E** ===> **H**



E

(3) →



H
YIELD 78%

RX(3) RCT E **228113-61-9**
RGT I 865-47-4 t-BuOK
PRO H **228113-62-0**
SOL 109-99-9 THF